Propanamide, N,N-diundecyl-3-cyclopentyl-

Inchi: InChI=1S/C30H59NO/c1-3-5-7-9-11-13-15-17-21-27-31(30(32)26-25-29-23-19-20-24-29)
InchiKey: PBPMNMAUVKULPK-UHFFFAOYSA-N
Formula: C30H59NO
SMILES: CCCCCCCCCCCN(CCCCCCCCCCC)C(=O)CCC1CCCC1
Mol. weight [g/mol]: 449.80

Physical Properties

Property code	Value	Unit	Source
gf	220.13	kJ/mol	Joback Method
hf	-647.10	kJ/mol	Joback Method
hfus	72.01	kJ/mol	Joback Method
hvap	91.42	kJ/mol	Joback Method
log10ws	-10.38		Crippen Method
logp	9.847		Crippen Method
mcvol	434.250	ml/mol	McGowan Method
pc	672.20	kPa	Joback Method
rinpol	3505.00		NIST Webbook
rinpol	3505.00		NIST Webbook
tb	967.39	K	Joback Method
tc	1191.22	K	Joback Method
tf	521.16	K	Joback Method
vc	1.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1555.13	J/mol×K	967.39	Joback Method
cpg	1580.50	J/mol×K	1004.69	Joback Method
cpg	1604.26	J/mol×K	1042.00	Joback Method
cpg	1626.52	J/mol×K	1079.30	Joback Method
cpg	1647.42	J/mol×K	1116.61	Joback Method
cpg	1667.08	J/mol×K	1153.91	Joback Method
cpg	1685.63	J/mol×K	1191.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308289&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume